



# Analytic Properties of Diffraction Gratings

Daniel Maystre

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# **GRATINGS: THEORY AND NUMERIC APPLICATIONS**

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Chapter 2:  
Analytic Properties of Diffraction Gratings  
Daniel Maystre

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## Chapter 2

# Analytic Properties of Diffraction Gratings

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### 2.1 Introduction

Since the 80's, specialists of gratings can rely on very powerful grating softwares [1-6]. These softwares are able to compute grating efficiencies for almost any kind of grating in any domain of wavelength, even though the progress of grating technologies needs endless extensions of grating theories to new kinds of structures. These softwares are based on elementary laws of Electromagnetics. Using mathematics, these laws lead to boundary value problems which can be solved on computers using adequate algorithms.

However, a grating user should not ignore some general properties of gratings which can be derived directly from the boundary value problem without any use of computer. These analytic properties are valuable at least for two reasons. First, they strongly contribute to a better understanding of an instrument which puzzled and fascinated many specialists of Optics since the beginning of the 20th century. Secondly, they allow a theoretician to check the validity of a new theory or its numerical implementation, although one must be very cautious: a theory can fail while its results satisfy some analytic rules. Specially, this surprising remark applies to properties like energy balance or reciprocity theorem.

The first part of this chapter is devoted to the use of the elementary laws of Electromagnetics for stating the boundary value problems of gratings in various cases of materials and polarizations. Then, we deduce from the boundary value problems the most important analytic properties of gratings.

### 2.2 From the laws of Electromagnetics to the boundary-value problems

#### 2.2.1 Presentation of the grating problem

Figure 2.1 represents a diffraction grating. Its periodic profile  $\mathcal{P}$  of period  $d$  along the  $x$  axis separates air (region  $\mathcal{R}_0$ ) from a grating material (region  $\mathcal{R}_1$ ) which is generally a metal or a dielectric. The  $y$  axis is the axis of invariance of the structure and the  $z$  axis is perpendicular to the average profile plane. We denote by  $z_M$  the ordinate of the top of  $\mathcal{P}$ , its bottom being located

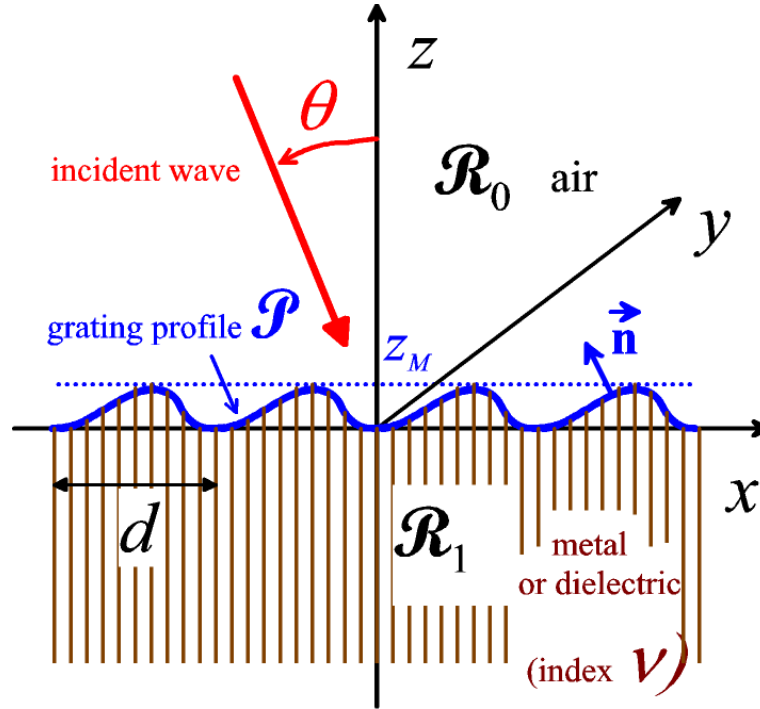


Figure 2.1: Notations.

on the  $xy$  plane by hypothesis. We suppose that the incident light can be described by a sum of monochromatic radiations of different frequencies. Each of these can in turn be described in a time-harmonic regime, which allows us to use the complex notation (with an  $\exp(-i\omega t)$  time-dependence). In this chapter, we assume that the wave-vector of each monochromatic radiation lies in the cross-section of the grating ( $xz$  plane). In the following, we deal with a single monochromatic radiation.

The electromagnetic properties of the grating material (assumed to be non-magnetic) are represented by its complex refractive index  $\nu$  which depends on the wavelength  $\lambda = 2\pi c/\omega$  in vacuum ( $c = 1/\sqrt{\epsilon_0\mu_0}$  being the speed of light, with  $\epsilon_0$  and  $\mu_0$  the permittivity and the permeability of vacuum). This complex index respectively includes the conductivity (for metals) and/or the losses (for lossy dielectrics). It becomes a real number for lossless dielectrics.

In the air region, the grating is illuminated by an incident plane wave. The incident electric field  $\vec{E}^i$  is given by :

$$\vec{E}^i = \vec{P} \exp(ik_0 x \sin(\theta) - ik_0 z \cos(\theta)), \quad (2.1)$$

with  $\theta$  being the angle of incidence, from the  $z$  axis to the incident direction, measured in the counterclockwise sense, and  $k_0$  being the wavenumber in the air ( $k_0 = 2\pi/\lambda$ , we take an index equal to unity for air). The wave-vector of the incident wave is given by:

$$\vec{k}_0^i = \begin{bmatrix} k_0 \sin(\theta) \\ 0 \\ -k_0 \cos(\theta) \end{bmatrix}. \quad (2.2)$$

The physical problem is to find the total electric and magnetic fields  $\vec{E}$  and  $\vec{H}$  at any point of space.

### 2.2.2 Maxwell's equations

First, let us notice that the physical problem remains unchanged after translations of the grating or of the incident wave along the  $y$  axis since they do not depend on  $y$ . Therefore, if  $\vec{E}(x, y, z)$  and  $\vec{H}(x, y, z)$  are the total fields for a given grating and a given incident wave,  $\vec{E}(x, y + y_0, z)$  and  $\vec{H}(x, y + y_0, z)$  will be solutions too, regardless of the value of  $y_0$ . Assuming, from the physical intuition, that the solution of the grating problem is unique, we deduce that  $\vec{E}$  and  $\vec{H}$  are independent of  $y$ .

In order to state the mathematical problem, we use the harmonic Maxwell equations in  $\mathcal{R}_0$ :

$$\nabla \times \vec{E} = i\omega\mu_0\vec{H}, \quad (2.3)$$

$$\nabla \times \vec{H} = -i\omega\varepsilon\vec{E}, \quad (2.4)$$

with:

$$\varepsilon = \begin{cases} \varepsilon_0 & \text{in } \mathcal{R}_0, \\ \varepsilon_1 = \varepsilon_0 v^2 & \text{in } \mathcal{R}_1. \end{cases} \quad (2.5)$$

In the following, equations (2.3) and (2.4) will be called first and second Maxwell equations respectively. We note that Maxwell's equations  $\nabla \cdot \vec{E} = 0$  and  $\nabla \cdot \vec{H} = 0$  are the straightforward consequences of the first and second Maxwell equations (it suffices to take the divergence of both members).

We introduce the diffracted fields  $\vec{E}^d$  and  $\vec{H}^d$  defined by:

$$\vec{E}^d = \begin{cases} \vec{E} - \vec{E}^i & \text{in } \mathcal{R}_0, \\ \vec{E} & \text{in } \mathcal{R}_1, \end{cases} \quad (2.6)$$

$$\vec{H}^d = \begin{cases} \vec{H} - \vec{H}^i & \text{in } \mathcal{R}_0, \\ \vec{H} & \text{in } \mathcal{R}_1. \end{cases} \quad (2.7)$$

The interest of the notion of diffracted field is that it satisfies the so-called **radiation condition** (or Sommerfeld condition, or outgoing wave condition), in contrast with the total field which does not satisfy this condition in  $\mathcal{R}_0$  since it includes the incident field. This means that the diffracted fields must remain bounded and propagate upwards in  $\mathcal{R}_0$  when  $z \rightarrow +\infty$ . The same property must be satisfied in  $\mathcal{R}_1$ , but that time the diffracted fields must remain bounded and propagate downwards in  $\mathcal{R}_1$  when  $z \rightarrow -\infty$ . Since the incident fields satisfy Maxwell's equations in  $\mathcal{R}_0$ , the diffracted fields satisfy these equations as well. Introducing the components of the diffracted fields on the three axes, Maxwell's equations yield:

$$\partial E_y^d / \partial z = -i\omega\mu_0 H_x^d, \quad (2.8a)$$

$$\partial E_y^d / \partial x = i\omega\mu_0 H_z^d, \quad (2.8b)$$

$$\partial E_z^d / \partial x - \partial E_x^d / \partial z = -i\omega\mu_0 H_y^d, \quad (2.8c)$$

$$\partial H_y^d / \partial z = i\omega\varepsilon E_x^d, \quad (2.9a)$$

$$\partial H_y^d / \partial x = -i\omega\varepsilon E_z^d, \quad (2.9b)$$

$$\partial H_z^d / \partial x - \partial H_x^d / \partial z = i\omega\varepsilon E_y^d. \quad (2.9c)$$



### 2.2.3 Boundary conditions on the grating profile

On the grating profile, the tangential component of the electric and magnetic fields must be continuous<sup>1</sup>. Thus the boundary condition is given by:

$$(\overrightarrow{[E^d]}_0 + \overrightarrow{[E^i]}_0) \times \overrightarrow{n} = \overrightarrow{[E^d]}_1 \times \overrightarrow{n}, \quad (2.10)$$

$$(\overrightarrow{[H^d]}_0 + \overrightarrow{[H^i]}_0) \times \overrightarrow{n} = \overrightarrow{[H^d]}_1 \times \overrightarrow{n}, \quad (2.11)$$

with  $\overrightarrow{n}$  being the unit normal to  $\mathcal{P}$ , oriented toward region  $\mathcal{R}_0$  (figure 2.1) and the symbol  $[\overrightarrow{F}]_p$  denoting the limit of  $\overrightarrow{F}$  when a point of region  $\mathcal{R}_p$  tends to the grating profile (with  $p \in (0, 1)$ ). As for Maxwell's equations, we note that the other boundary conditions on the normal components of the fields are consequences of equations (2.10) and (2.11). It is worth noting that the linkage between these two boundary conditions is a typical example of an elementary property which is difficult to establish, at least for those who are not acquainted with the theory of distributions. Projecting equations (2.10) and (2.11) on the three axes yields:

$$[E_y^d]_0 - [E_y^d]_1 = -[E_y^i]_0, \quad (2.12a)$$

$$n_x[E_z^d]_0 - n_z[E_x^d]_0 - n_x[E_z^d]_1 + n_z[E_x^d]_1 = -n_x[E_z^i]_0 + n_z[E_x^i]_0, \quad (2.12b)$$

$$[H_y^d]_0 - [H_y^d]_1 = -[H_y^i]_0, \quad (2.13a)$$

$$n_x[H_z^d]_0 - n_z[H_x^d]_0 - n_x[H_z^d]_1 + n_z[H_x^d]_1 = -n_x[H_z^i]_0 + n_z[H_x^i]_0. \quad (2.13b)$$

### 2.2.4 Separating the general boundary-value problem into two separated scalar problems

The first conclusion to draw from equations (2.8), (2.9), (2.12) and (2.13) is that **they can be separated into two independent sets**. The first one, called TE case, includes equations (2.8a), (2.8b), (2.9c), (2.12a) and (2.13b). It only contains the transverse component (viz. the y-component)  $E_y^d$  of the electric field and the  $xz$  components (orthogonal to the y axis)  $H_x^d$  and  $H_z^d$  of the magnetic field. It must be remembered that the incident field  $\overrightarrow{E^i}$  is given by equation (2.1) and thus is not an unknown field. The same remark applies to the complementary set (TM case), but with the transverse component of the magnetic field and the  $xz$  components of the electric field. As a consequence, the general problem of diffraction by a grating can be decomposed into two elementary mathematical problems.

#### 2.2.4.1 The TE case problem

In the first one, the  $xz$  components of the magnetic field can be expressed as functions of the transverse component of the electric field using equations (2.8a) and (2.8b). Inserting their expression in equation (2.9c) shows that  $E_y^d$  satisfies a Helmholtz equation:

$$\boxed{\nabla^2 E_y^d + k^2 E_y^d = 0,} \quad (2.14)$$

<sup>1</sup>The continuity of the tangential component of the magnetic field is valid for materials having bounded values of permittivity. When the permittivity of the grating material is infinite, as in the model of perfectly conducting material, this condition does not hold.

with:

$$k = \begin{cases} k_0 & \text{in } \mathcal{R}_0, \\ k_1 = k_0 v & \text{in } \mathcal{R}_1. \end{cases} \quad (2.15)$$

The associated boundary condition on the diffracted electric field can be deduced from equations (2.12a) and (2.1):

$$\boxed{\left[ E_y^d \right]_0 - \left[ E_y^d \right]_1 = -P_y \exp(ik_0 x \sin(\theta) - ik_0 z \cos(\theta)), \quad \text{with } (x, z) \in \mathcal{P},} \quad (2.16)$$

while the associated boundary condition on its normal derivative can be deduced from equations (2.13b), (2.8a) and (2.8b):

$$\boxed{\begin{aligned} \left[ \frac{dE_y^d}{dn} \right]_0 - \left[ \frac{dE_y^d}{dn} \right]_1 &= - \left[ \frac{dE_y^i}{dn} \right]_0, \\ &= -iP_y \vec{n} \cdot \vec{k}_0^i \exp(ik_0 x \sin(\theta) - ik_0 z \cos(\theta)), \quad \text{with } (x, z) \in \mathcal{P}, \end{aligned}} \quad (2.17)$$

with  $\frac{dF}{dn}$  denoting the normal derivative  $\vec{n} \cdot \nabla F$ . It can be noticed that equation (2.17) entails the continuity of the normal derivative of the transverse component of the total electric field. Equations (2.14), (2.16) and (2.17) are not sufficient to define the boundary-value problem for TE case. A fourth condition must be added: the radiation condition:

$$\boxed{E_y^d \text{ must satisfy a radiation condition for } z \rightarrow \pm\infty.} \quad (2.18)$$

The boundary value problem allows us to deduce a fundamental property of gratings. Let us suppose that the incident field is TE polarized, i.e. that the electric incident field is parallel to the  $y$  axis ( $P_x = P_z = 0$ ). In these conditions, the equations associated with the TM case are homogeneous: they do not contain the incident field since the right-hand member of equation (2.12b) vanishes. If we believe that the solution of the grating problem is unique, it must be concluded that the  $xz$  component of the diffracted and total electric field vanish. On the other hand, the magnetic field is parallel to the  $xz$  plane. In other words, **in the TE case, the grating problem becomes scalar: we must determine the  $y$ -component of the diffracted electric field**. The  $xz$  components of the magnetic field deduce the  $y$ -component of the diffracted electric field using equations (2.8a) and (2.8b).

#### 2.2.4.2 The TM case problem

Now, let us deal with the TM case. As for the TE case, it can be shown that the  $y$ -component of the magnetic field satisfies a Helmholtz equation by using equations (2.8c), (2.9a) and (2.9b):

$$\boxed{\nabla^2 H_y^d + k^2 H_y^d = 0.} \quad (2.19)$$

The boundary conditions need the calculation of the incident magnetic field. From equation (2.1) and Maxwell equation (2.3), it turns out that:

$$\vec{H}^i = \vec{Q} \exp(ik_0 x \sin(\theta) - ik_0 z \cos(\theta)), \quad (2.20)$$

with:

$$\vec{Q} = \frac{1}{\omega\mu_0} \vec{k}_0^t \cdot \vec{P} \exp(ik_0x \sin(\theta) - ik_0z \cos(\theta)). \quad (2.21)$$

The associated boundary condition on the diffracted magnetic field can be deduced from equations (2.13a) and (2.20):

$$[H_y^d]_0 - [H_y^d]_1 = -Q_y \exp(ik_0x \sin(\theta) - ik_0z \cos(\theta)), \quad \text{with } (x, z) \in \mathcal{P}, \quad (2.22)$$

while the boundary condition on its normal derivative is obtained by inserting the expressions of the  $xz$  components of the electric field (equations (2.9a) and (2.9b)) in equation (2.12b). Remarking that the incident field satisfies the same equations, we obtain finally:

$$\begin{aligned} \frac{1}{\varepsilon_0} \left[ \frac{dH_y^d}{dn} \right]_0 - \frac{1}{\varepsilon_1} \left[ \frac{dH_y^d}{dn} \right]_1 &= -\frac{1}{\varepsilon_0} \left[ \frac{dH_y^i}{dn} \right]_0, \\ &= -\frac{iQ_y}{\varepsilon_0} \vec{n} \cdot \vec{k}_0^i \exp(ik_0x \sin(\theta) - ik_0z \cos(\theta)), \quad \text{with } (x, z) \in \mathcal{P}. \end{aligned} \quad (2.23)$$

It can be noticed that equation (2.23) has a simple interpretation: the product  $\frac{1}{\varepsilon} \frac{dH_y}{dn}$  is continuous across the profile. Finally, the radiation condition yields:

$$H_y^d \text{ must satisfy a radiation condition for } z \rightarrow \pm\infty. \quad (2.24)$$

Equations (2.19), (2.22), (2.23) and radiation conditions for  $z \rightarrow \pm\infty$  define the boundary-value problem for TM case. As for TE case, the uniqueness of the solution shows that when the magnetic incident field is parallel to the  $y$  axis ( $Q_x = Q_z = 0$ ), the equations associated with the TE case are homogeneous: they do not contain the incident field. It can be concluded that the  $xz$  components of the diffracted and total magnetic fields vanish. On the other hand, the electric field is parallel to the  $xz$  plane. In other words, **in the TM case, the grating problem becomes scalar: we must determine the  $y$ -component of the diffracted magnetic field**. The  $xz$  components of the electric field deduce from the  $y$ -component of the diffracted magnetic field using equations (2.9a) and (2.9b).

### 2.2.4.3 TE and TM cases: a unified presentation of the boundary-value problem

In order to deal with both cases simultaneously, we denote by  $F^d$  the field defined by:

$$F^d = \begin{cases} E_y^d & \text{for TE case,} \\ H_y^d & \text{for TM case.} \end{cases} \quad (2.25)$$

In the same way, by assuming that the incident field has a unit amplitude ( $P_y=1$  for TE case and  $Q_y=1$  for TM case), the incident field in both cases is given by:

$$F^i = \exp(ik_0x \sin(\theta) - ik_0z \cos(\theta)), \quad (2.26)$$

the total field  $F$  being given by:

$$F = \begin{cases} F^d + F^i & \text{in } \mathcal{R}_0, \\ F^d & \text{in } \mathcal{R}_1. \end{cases} \quad (2.27)$$

Using equations (2.14), (2.16), (2.17), (2.18), (2.19), (2.22), (2.23) and (2.24), it is possible to gather both cases in a unique set of equations:

$$\nabla^2 F^d + k^2 F^d = 0, \quad (2.28)$$

$$\left[ F^d \right]_0 - \left[ F^d \right]_1 = -\exp(ik_0 x \sin(\theta) - ik_0 z \cos(\theta)) \quad \text{with } (x, z) \in \mathcal{P}, \quad (2.29)$$

$$\frac{1}{\tau_0} \left[ \frac{dF^d}{dn} \right]_0 - \frac{1}{\tau_1} \left[ \frac{dF^d}{dn} \right]_1, \quad (2.30)$$

$$= -\frac{i}{\tau_0} \vec{n} \cdot \vec{k}_0^t \exp(ik_0 x \sin(\theta) - ik_0 z \cos(\theta)), \quad \text{with } (x, z) \in \mathcal{P},$$

$$F^d \text{ must satisfy a radiation condition for } y \rightarrow \pm\infty, \quad (2.31)$$

with:

$$\tau_i = \begin{cases} 1 & \text{for TE case,} \\ \varepsilon_i & \text{for TM case, } i \in (0, 1). \end{cases} \quad (2.32)$$

In the following, this boundary-value problem will be called normalized grating problem. It is worth noting that equations (2.29) and (2.30) take a simpler form by introducing the total field  $F$ :

$$[F]_0 = [F]_1, \quad (2.33)$$

$$\frac{1}{\tau_0} \left[ \frac{dF}{dn} \right]_0 = \frac{1}{\tau_1} \left[ \frac{dF}{dn} \right]_1. \quad (2.34)$$

### 2.2.5 The special case of the perfectly-conducting grating

The first grating theories were devoted to perfectly conducting gratings. This case is very important since it is realistic for metallic gratings in the microwave domain and far infrared regions. In the visible and infrared regions, it can provide qualitative results. However, in these regions, one must be very cautious. The existence of surface plasmons propagating at the vicinity of the grating surface generates strong resonance phenomena for TM case. **Due to these phenomena, the properties of real metallic gratings and those of perfectly-conducting gratings may completely differ** [2]. Moreover, the perfect conductivity model allows one to simplify the grating theory, since the associated boundary-value problems are much simpler.

Basically, the equations associated to the perfect conductivity model are the same as for real metallic or dielectric gratings, except equations (2.4) and (2.11). Let us give a brief explanation to this property. In Maxwell equation (2.4), the right-hand member includes the volume current density  $\vec{j}$  in the metal since this term is proportional to the electric field ( $\vec{j} = \sigma \vec{E}$ ,  $\sigma$  being the conductivity of the metal). When the conductivity tends to infinity, the volume current density and the total fields concentrate more and more on the grating surface since the skin depth tends to zero. As a consequence, at the limit when the conductivity tends to infinity, the fields are null in  $\mathcal{R}_1$  while the volume current density  $\vec{j}$  becomes a surface current density  $\vec{j}_{\mathcal{P}}$ . This surface current density cannot be included in the right-hand member of equation (2.4) since it is a singular distribution (for the specialist of Schwartz distributions [7], it writes  $\vec{j}_{\mathcal{P}} \delta_{\mathcal{P}}$ ). Finally, equation (2.4) becomes:

$$\nabla \times \vec{H} = -i\omega \tilde{\epsilon} \vec{E} + \vec{j}_{\mathcal{P}}, \quad (2.35)$$

with  $\tilde{\epsilon}$  being the permittivity of the material. Furthermore, taking into account that the total fields vanish inside  $\mathcal{R}_1$ , the boundary condition (equation (2.11)) becomes:

$$\vec{n} \times (\overrightarrow{[H^d]}_0 + \overrightarrow{[H^i]}_0) = \vec{j}_{\mathcal{P}}. \quad (2.36)$$

This equation reduces to a relation between the surface current density on  $\mathcal{P}$  and the limit of the magnetic field above  $\mathcal{P}$ . It does not constitute any more an element of the boundary-value problem.

In conclusion, for perfectly conducting gratings, the fields inside  $\mathcal{R}_1$  vanish and, using equations (2.3), (2.4), (2.10), (2.6) and (2.7), the basic vector equations for the field in  $\mathcal{R}_0$  can be written:

$$\nabla \times \overrightarrow{E^d} = i\omega\mu_0\overrightarrow{H^d}, \quad (2.37)$$

$$\nabla \times \overrightarrow{H^d} = -i\omega\epsilon_0\overrightarrow{E^d}, \quad (2.38)$$

$$(\overrightarrow{[E^d]}_0 + \overrightarrow{[E^i]}_0) \times \vec{n} = 0. \quad (2.39)$$

Following the same lines as in subsections 2.2.4.1 and 2.2.4.2, the boundary value problems for perfectly conducting gratings are given by:

For TE case:

$$\nabla^2 E_y^d + k_0^2 E_y^d = 0, \quad (2.40)$$

$$\left[ E_y^d \right]_0 = -P_y \exp(ik_0 x \sin(\theta) - ik_0 z \cos(\theta)), \quad \text{with } (x, z) \in \mathcal{P}, \quad (2.41)$$

$$E_y^d \text{ must satisfy a radiation condition for } z \rightarrow +\infty. \quad (2.42)$$

For TM case:

$$\nabla^2 H_y^d + k_0^2 H_y^d = 0, \quad (2.43)$$

$$\left[ \frac{dH_y^d}{dn} \right]_0 = -iQ_y \vec{n} \cdot \vec{k}_0 \exp(ik_0 x \sin(\theta) - ik_0 z \cos(\theta)), \quad \text{with } (x, z) \in \mathcal{P}, \quad (2.44)$$

$$H_y^d \text{ must satisfy a radiation condition for } z \rightarrow +\infty. \quad (2.45)$$

### 2.3 Pseudo-periodicity of the field and Rayleigh expansion

This section establishes the most famous property of diffraction gratings: the dispersion of light, which is a consequence of the well known grating formula. In general, this formula is demonstrated using heuristic considerations of physical optics. Here, we propose a rigorous demonstration based on the boundary-value problem stated in subsection 2.2.4.3. First, let us show that the field  $F^d$  is pseudo-periodic, i.e. that:

$$F^d(x + d, z) = F^d(x, z) \exp(ik_0 d \sin(\theta)). \quad (2.46)$$

With this aim, we consider the function  $G(x, z)$  defined by:

$$G(x, z) = F^d(x + d, z) \exp(-ik_0 d \sin(\theta)). \quad (2.47)$$

The pseudo-periodicity of  $F^d$  is proved if we show that  $F^d(x, z) = G(x, z)$ . Owing to the uniqueness of the solution of the boundary-value problem defined by equations (2.28), (2.29), (2.30) and (2.31), this equation is satisfied if  $G$  obeys the same equations. Obviously,  $G$  satisfies these equations since  $d$  is the grating period. Thus  $F^d$  is pseudo-periodic, with coefficient of pseudo-periodicity  $k_0 \sin(\theta)$ , as well as  $F^i$  and  $F$ . Notice that in normal incidence ( $\theta = 0$ ), pseudo-periodicity becomes ordinary periodicity, which in that case is a straightforward property since both grating and incident wave are periodic.

Using the pseudo-periodicity, let us show that the field above and below the grating is a sum of plane waves. With this aim, we notice from equation (2.28) that  $F^d(x, z) \exp(-ik_0 x \sin(\theta))$  has a period  $d$  and thus can be expanded in a Fourier series:

$$F^d(x, z) \exp(-ik_0 x \sin(\theta)) = \sum_{n=-\infty}^{+\infty} F_n^d(z) \exp(2i\pi n x/d). \quad (2.48)$$

Multiplying both members of equation (2.48) by  $\exp(ik_0 x \sin(\theta))$  yields :

$$F^d(x, z) = \sum_{n=-\infty}^{+\infty} F_n^d(z) \exp(i\alpha_n x), \quad (2.49)$$

with:

$$\alpha_n = k_0 \sin(\theta) + 2\pi n/d. \quad (2.50)$$

Introducing this expression of  $F^d(x, z)$  in Helmholtz equation (2.28), we find :

$$\sum_{n=-\infty}^{+\infty} (d^2 F_n^d(z)/dz^2 + (k^2 - \alpha_n^2) F_n^d(z)) \exp(i\alpha_n x) = 0, \quad (2.51)$$

and multiplying both members by  $\exp(-ik_0 x \sin(\theta))$ ,

$$\sum_{n=-\infty}^{+\infty} (d^2 F_n^d(z)/dz^2 + (k^2 - \alpha_n^2) F_n^d(z)) \exp(2i\pi n x/d) = 0. \quad (2.52)$$

It seems, at the first glance, that the left-hand member of equation (2.52) is a Fourier series, and thus that the coefficients of this Fourier series vanish. This is not correct. Indeed, we have to bear in mind that  $k$ , defined in equation (2.15) is not a constant. As a consequence, if  $0 < y < z_M$ , a region called intermediate region in the following,  $k^2$  depends on  $x$  and the left-hand member of equation (2.52) is not a Fourier series. However, above and below this intermediate region,  $k^2$  is constant and we can write that the Fourier coefficients vanish:

$$\forall n, \quad d^2 F_n^d(z)/dz^2 + \gamma_{0,n}^2 F_n^d(z) = 0 \quad \text{if } y > z_M, \quad (2.53a)$$

$$\forall n, \quad d^2 F_n^d(z)/dz^2 + \gamma_{1,n}^2 F_n^d(z) = 0 \quad \text{if } y < 0, \quad (2.53b)$$

with:

$$\gamma_{i,n} = \sqrt{(k_i^2 - \alpha_n^2)} \quad i \in (0, 1). \quad (2.54)$$

We deduce that:

$$F_n^d(z) = \begin{cases} I_{0,n} \exp(-i\gamma_{0,n} z) + D_{0,n} \exp(+i\gamma_{0,n} z) & \text{if } y > z_M, \\ D_{1,n} \exp(-i\gamma_{1,n} z) + I_{1,n} \exp(+i\gamma_{1,n} z) & \text{if } y < 0, \end{cases} \quad (2.55)$$

and therefore, using equation (2.49),

$$F^d(x, z) = \begin{cases} \sum_{n=-\infty}^{+\infty} (I_{0,n} \exp(i\alpha_n x - i\gamma_{0,n} z) + D_{0,n} \exp(i\alpha_n x + i\gamma_{0,n} z)) & \text{if } z > z_M, \\ \sum_{n=-\infty}^{+\infty} (D_{1,n} \exp(i\alpha_n x - i\gamma_{1,n} z) + I_{1,n} \exp(i\alpha_n x + i\gamma_{1,n} z)) & \text{if } z < 0. \end{cases} \quad (2.56)$$

Let us remark that equation (2.54) does not assign to  $\gamma_{i,n}$  a unique value. However, equation (2.56) shows that its determination can be chosen arbitrarily since a sign change does not modify the value of the field, provided that  $I_{0,n}$  and  $D_{0,n}$  are permuted. The determination of these constants will be given by:

$$\operatorname{Re}(\gamma_{i,n}) + \operatorname{Im}(\gamma_{i,n}) > 0, \quad i \in (0, 1), \quad (2.57)$$

with  $\operatorname{Re}(q)$  and  $\operatorname{Im}(q)$  denoting the real and imaginary parts of  $q$ .

Equation (2.56) shows that the field above and below the intermediate region can be represented by plane wave expansions. The propagation constants of the plane waves along the  $x$  and  $z$  axes are respectively equal to  $\alpha_n$  and  $\pm\gamma_{i,n}$ . In the physical problem, some of these plane waves must be rejected since they do not obey the radiation condition. This condition entails that  $I_{0,n} = I_{1,n} = 0$  since, according to equation (2.57), the associated plane waves propagate towards the grating profile. Finally, equations (2.56), (2.27) and the radiation condition allow us to express the total field by adding the incident field:

$$F(x, z) = \begin{cases} \exp(i\alpha_0 x - i\gamma_{0,0} z) + \sum_{n=-\infty}^{+\infty} D_{0,n} \exp(i\alpha_n x + i\gamma_{0,n} z) & \text{if } z > z_M, \\ \sum_{n=-\infty}^{+\infty} D_{1,n} \exp(i\alpha_n x - i\gamma_{1,n} z) & \text{if } z < 0, \end{cases} \quad (2.58)$$

the sums being the expression of the scattered field in both regions. The unknown complex coefficients  $D_{0,n}$  and  $D_{1,n}$  are the amplitudes of the reflected and transmitted waves respectively.

**The conclusion of this subsection is that above and below the intermediate region, the field reflected and transmitted by the grating takes the form of sums of plane waves (Rayleigh expansion [8]), each of them being characterized by its order  $n$ .**

## 2.4 Grating formulae

According to equation (2.54), almost all the diffracted plane waves (an infinite number) are evanescent: they propagate along the  $x$  axis at the vicinity of the grating profile since they decrease exponentially when  $|z| \rightarrow +\infty$ . For  $z \rightarrow +\infty$ , they correspond to the orders  $n$  such that  $\alpha_n^2 \geq k_0^2$ , thus rendering  $\gamma_{0,n} = i\sqrt{(\alpha_n^2 - k_0^2)}$  a purely imaginary number. Only a finite number of them, called  $z$ -propagative orders, propagate towards  $z = +\infty$ , with  $\alpha_n^2 \leq k_0^2$ , thus  $\gamma_{0,n} = \sqrt{(k_0^2 - \alpha_n^2)}$  being real. Let us notice that among these orders, the  $0^{th}$  order is always included, since  $\gamma_{0,n} = k_0 \cos(\theta)$ . It propagates in the direction specularly reflected by the mean plane of the profile, whatever the wavelength may be. In contrast, the other  $z$ -propagative orders are dispersive. Indeed, their propagation constants along the  $x$  and  $z$  axes are equal to  $\alpha_n$  and  $\gamma_{0,n}$ , in such a way that the diffraction angle  $\theta_{0,n}$  of one of these waves, measured clockwise from the  $z$  axis, can be deduced from  $\alpha_n = k_0 \sin(\theta_{0,n})$ . Using the expression of  $\alpha_n$  given by equation (2.50), the angle of diffraction is given by :

$$\boxed{\sin(\theta_{0,n}) = \sin(\theta) + n \frac{2\pi}{k_0 d} = \sin(\theta) + n \frac{\lambda}{d}.} \quad (2.59)$$

This is the famous grating formula, often deduced from heuristic arguments of physical optics.

For the field below the grooves, the wavenumber  $k_0$  is replaced by  $k_1 = k_0 v$ . If the grating material is a lossless dielectric, the directions of propagation of the transmitted field obey a grating formula as well. This formula is similar to equation (2.59) but the angles of transmission  $\theta_{1,n}$  can be deduced from  $\alpha_n = k_0 v \sin(\theta_{1,n})$ , which yields, using a counterclockwise convention:

$$v \sin(\theta_{0,n}) = \sin(\theta) + n \frac{2\pi}{k_0 d} = \sin(\theta) + n \frac{\lambda}{d}. \quad (2.60)$$

The  $0^{th}$  order is always included in the  $z$ -propagative orders<sup>2</sup>. It propagates in the direction of transmission by an air/dielectric plane interface, whatever the wavelength may be. In contrast, the other  $z$ -propagative orders are dispersive. When the grating material is metallic, the transmitted plane waves are absorbed by the metal and the  $z$ -propagating orders below the grooves no longer exist.

In conclusion of this section, **the reflected and transmitted fields include, outside the grooves, a finite number of plane waves propagating to infinity with scattering angles given by the grating formulae. All the orders are dispersive, except the  $0^{th}$  orders.** The reflected  $0^{th}$  order takes the specular direction while for a lossless material, the transmitted  $0^{th}$  order takes the direction transmitted by an air/dielectric plane interface. **Consequently, a polychromatic incident plane wave generates in a given order  $n$  different from 0 a sum of plane waves scattered in different directions, i.e. a spectrum.** The measurement of the intensity along this spectrum allows one to determine the spectral power of the incident wave. This dispersion phenomenon is the most important property of diffraction gratings. It explains why this optical component has been one of the most valuable tools in the history of Science.

## 2.5 Analytic properties of gratings

### 2.5.1 Balance relations

The mathematical balance relations established in this subsection will allow us to demonstrate very important general properties of gratings. These balance relations state mathematical links between characteristics of the field in two regions separated by large distances, without considering the fields in between. They can give a relation between the fields at  $z = +\infty$  and the fields on the grating profile, or the fields at  $z = -\infty$  and the fields on the grating profile, or the fields at  $z = +\infty$  and  $z = -\infty$ .

#### 2.5.1.1 Lemma 1

We consider two pseudoperiodic functions  $u$  and  $v$  of the two variables  $x$  and  $z$ , defined in  $\mathcal{R}_0$ , which belong to the class  $G_0$  of functions having the following properties:

- They are pseudo-periodic, with the same coefficient of pseudo-periodicity  $\alpha$ , in other words,  $u(x, z) \exp(-i\alpha x)$  and  $v(x, z) \exp(-i\alpha x)$  are periodic,

<sup>2</sup>This property does not hold if the upper medium is not air but has an index  $\tilde{v}$  greater than the index  $v$  of the lower medium, provided that the incidence is chosen in such a way that the incident wave is totally reflected by a plane interface (Total Internal Reflection). In that case,  $\sin(\theta)$  is replaced by  $\tilde{v} \sin(\theta)$  in equation (2.60), in such a way that the zeroth order is evanescent if  $\tilde{v} \sin(\theta) > v$ .



- They are solutions of a Helmholtz equation:

$$\nabla^2 u + k_0^2 u = 0, \quad (2.61a)$$

$$\nabla^2 v + k_0^2 v = 0, \quad (2.61b)$$

with  $k_0$  being real.

- They are bounded for  $z \rightarrow \infty$ ,
- They are square integrable in  $x$  and locally square integrable in  $z$ ,
- Their values on  $\mathcal{P}$  are square integrable, as well as their normal derivatives.

We introduce the sesquilinear functional defined by:

$$\mathcal{F}_0 = \int_{\mathcal{P}} \left( u \frac{d\bar{v}}{dn} - \bar{v} \frac{du}{dn} \right) ds. \quad (2.62)$$

The symbol  $\int_{\mathcal{P}}$  denotes a curvilinear integral on one period of the profile  $\mathcal{P}$  of the grating, with  $ds$  being the differential of the curvilinear abscissa on  $\mathcal{P}$ . Obviously, the value in region  $\mathcal{R}_0$  of the fields  $F(x, z)$ , solutions of the four boundary-value problems defined in subsection 2.2.4, belong to  $G_0$ , as well as the incident field  $F^i$ . It is to be noticed that we do not impose a boundary condition on  $\mathcal{P}$  or a radiation condition at infinity, but we still impose that these functions must remain bounded at infinity.

Following the same lines as in section 2.3, it can be shown that above the top of the grooves,  $u$  and  $v$  can be represented by plane wave expansions, similar to that of equation (2.56): if  $z > z_M$ ,

$$u(x, z) = \sum_{n=-\infty}^{+\infty} [I_{0,n} \exp(i\alpha_n x - i\gamma_{0,n} z) + D_{0,n} \exp(i\alpha_n x + i\gamma_{0,n} z)], \quad (2.63a)$$

$$v(x, z) = \sum_{n=-\infty}^{+\infty} [I'_{0,n} \exp(i\alpha_n x - i\gamma_{0,n} z) + D'_{0,n} \exp(i\alpha_n x + i\gamma_{0,n} z)]. \quad (2.63b)$$

Let us notice that some terms must be eliminated in the Rayleigh expansions. Indeed, the field must remain bounded at infinity. It is not the case for the incident terms of coefficients  $I_{0,n}$  and  $I'_{0,n}$  unless the corresponding plane waves are  $z$ -propagating waves. Thus we define the set  $U_0$  of orders corresponding to  $z$ -propagating waves and equations (2.63) become:

$$u(x, z) = \sum_{n \in U_0} I_{0,n} \exp(i\alpha_n x - i\gamma_{0,n} z) + \sum_{n=-\infty}^{+\infty} D_{0,n} \exp(i\alpha_n x + i\gamma_{0,n} z), \quad (2.64a)$$

$$v(x, z) = \sum_{n \in U_0} I'_{0,n} \exp(i\alpha_n x - i\gamma_{0,n} z) + \sum_{n=-\infty}^{+\infty} D'_{0,n} \exp(i\alpha_n x + i\gamma_{0,n} z), \quad (2.64b)$$

$$\begin{aligned} \overline{v(x, z)} &= \sum_{n \in U_0} \overline{I'_{0,n}} \exp(-i\alpha_n x + i\gamma_{0,n} z) + \\ &\quad + \sum_{n=-\infty}^{+\infty} \overline{D'_{0,n}} \exp(-i\alpha_n x - i\gamma_{0,n} z). \end{aligned} \quad (2.64c)$$

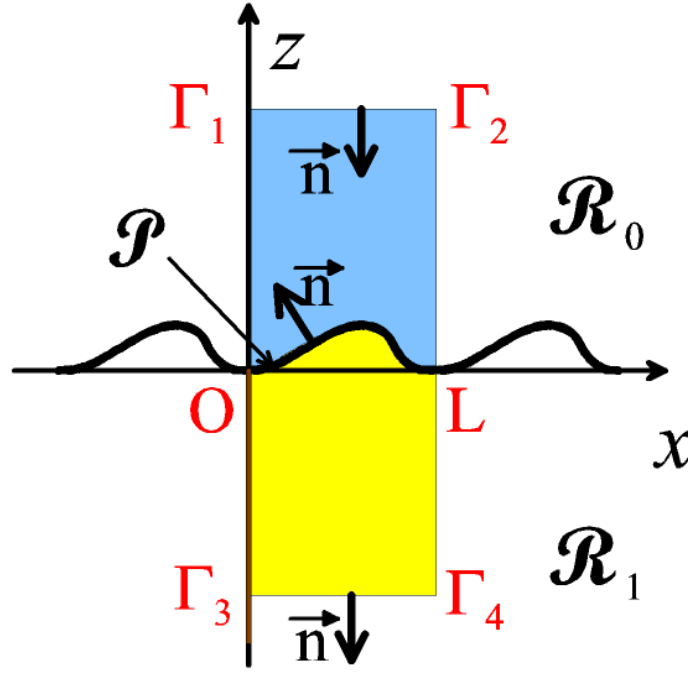


Figure 2.2: Balance relations.

Now, we show that  $\mathcal{F}_0$  can be expressed as a function of the Rayleigh coefficients  $I_{0,n}$ ,  $D_{0,n}$ ,  $I'_{0,n}$  and  $D'_{0,n}$ . With this aim, we multiply equation (2.61a) by  $\bar{v}$ , the conjugate of equation (2.61b) by  $u$  and we subtract the first from the second, which yields:

$$u\nabla^2\bar{v} - \bar{v}\nabla^2u = 0 \quad \text{in } \mathcal{R}_0. \quad (2.65)$$

Integrating equation (2.65) in the blue area of figure 2.2 and applying the second Green identity yields:

$$\int_{\Omega_0} \left( u \frac{d\bar{v}}{dn} - \bar{v} \frac{du}{dn} \right) dl = 0, \quad (2.66)$$

with  $\Omega_0$  being the boundary of the blue area of figure 2.2 and  $dl$  denoting the differential of the curvilinear abscissa on  $\Omega_0$ . According to equations (2.64a) and (2.64c),  $u \frac{d\bar{v}}{dx}$  and  $\bar{v} \frac{du}{dx}$  are periodic. Since the orientations of the normal on verticals  $O\Gamma_1$  and  $L\Gamma_2$  are opposite, the contributions of the integrals on these segments cancel each other. Furthermore, the normal to  $O\Gamma_1$  and  $L\Gamma_2$  is parallel to the  $z$  axis and oriented downwards, then equation (2.66) becomes:

$$\int_{\mathcal{P}} \left( u \frac{d\bar{v}}{dn} - \bar{v} \frac{du}{dn} \right) ds = \int_{\Gamma_1\Gamma_2} \left( u \frac{d\bar{v}}{dz} - \bar{v} \frac{du}{dz} \right) dx. \quad (2.67)$$

Introducing in the right-hand member of equation (2.66) the expressions of  $u$  and  $\bar{v}$  given by equations (2.64a) and (2.64c), separating the terms  $n \in U_0$  from the other ones and taking into account that  $\int_{x=0}^d \exp(in\frac{2\pi}{d}x) = \delta_{n,0}$ , with  $\delta_{n,0}$  being the Kronecker symbol, one can obtain, after some cumbersome but not difficult calculations that:

$$\boxed{\int_{\mathcal{P}} \left( u \frac{d\bar{v}}{dn} - \bar{v} \frac{du}{dn} \right) ds = \sum_{n \in U_0} \gamma_{0,n} (I_{0,n} \overline{I'_{0,n}} - D_{0,n} \overline{D'_{0,n}}).} \quad (2.68)$$

### 2.5.1.2 Lemma 2

In this section, it is supposed that the grating material is lossless, in such a way that plane waves can propagate in  $\mathcal{R}_1$ . Lemma 2 is similar as lemma 1, but for region  $\mathcal{R}_1$ . We denote by  $U_1$  the set of orders corresponding to  $z$ -propagating waves in  $\mathcal{R}_1$ . The expressions of  $u$  and  $v$  below the  $x$  axis are given by:

$$u(x, z) = \sum_{n \in U_1} D_{1,n} \exp(i\alpha_n x - i\gamma_{1,n} z) + \sum_{n=-\infty}^{+\infty} I_{1,n} \exp(i\alpha_n x + i\gamma_{1,n} z), \quad (2.69a)$$

$$v(x, z) = \sum_{n \in U_1} D'_{1,n} \exp(i\alpha_n x - i\gamma_{1,n} z) + \sum_{n=-\infty}^{+\infty} I'_{1,n} \exp(i\alpha_n x + i\gamma_{1,n} z), \quad (2.69b)$$

$$\begin{aligned} \overline{v(x, z)} = \sum_{n \in U_1} \overline{D'_{1,n}} \exp(-i\alpha_n x + i\gamma_{1,n} z) + \\ + \sum_{n=-\infty}^{+\infty} \overline{I'_{1,n}} \exp(-i\alpha_n x - i\gamma_{1,n} z). \end{aligned} \quad (2.69c)$$

Following the same lines as in section 2.5.1.1 but for the yellow area of figure 2.2 and noting that the normal is now oriented towards the exterior of the domain, it can be deduced that:

$$\int_{\mathcal{P}} \left( u \frac{d\bar{v}}{dn} - \bar{v} \frac{du}{dn} \right) ds = - \sum_{n \in U_1} \gamma_{1,n} (I_{1,n} \overline{I'_{1,n}} - D_{1,n} \overline{D'_{1,n}}). \quad (2.70)$$

### 2.5.2 Compatibility between Rayleigh coefficients

In order to state a relation between the Rayleigh coefficients above and below the grating profile, we assume that the functions  $u$  and  $v$  satisfy the boundary conditions imposed on the total fields by equations (2.33) and (2.34). On the other hand, we do not impose radiation conditions at infinity, but the functions must remain bounded. In other words,  $u$  and  $v$  can be considered as solutions of the most general grating problem, in which the incident wave is not restricted to a single plane wave, but to the sum of all the plane waves generating diffracted waves in the same directions, with arbitrary amplitudes. It is straightforward to show from equations (2.33) and (2.34) that the left-hand members of equations (2.68) and (2.70) are proportional, then to deduce a relation including the coefficients of the Rayleigh expansions of the field only:

$$\begin{aligned} \frac{1}{\tau_0} \sum_{n \in U_0} \gamma_{0,n} (I_{0,n} \overline{I'_{0,n}} - D_{0,n} \overline{D'_{0,n}}) + \\ \frac{1}{\tau_1} \sum_{n \in U_1} \gamma_{1,n} (I_{1,n} \overline{I'_{1,n}} - D_{1,n} \overline{D'_{1,n}}) = 0. \end{aligned} \quad (2.71)$$

This equation states the most general relation of compatibility between two solutions of the general diffraction grating problem associated to different sets of incident waves. When the grating material is perfectly conducting, it is easy to show that the compatibility equation holds, provided that the sum  $n \in U_1$  is cancelled in equation (2.71).

Phenomenological theories of gratings make a wide use of the notion of scattering matrix (or  $S$ -matrix). The scattering matrix states the linear relation between the amplitudes of the diffracted and incident waves. We define the column matrix containing the amplitudes of the incident waves. More precisely, we define the normalized amplitudes of the incident and scattered waves by  $\tilde{I}_{0,n} = \sqrt{\gamma_{0,n}} I_{0,n}$ ,  $\tilde{D}_{0,n} = \sqrt{\gamma_{0,n}} D_{0,n}$ ,  $\tilde{I}_{1,n} = \sqrt{\frac{\tau_0}{\tau_1}} \gamma_{1,n} I_{1,n}$ ,  $\tilde{D}_{1,n} = \sqrt{\frac{\tau_0}{\tau_1}} \gamma_{1,n} D_{1,n}$ ,  $n \in (0, 1)$ , and by definition, the scattering matrix is a square matrix defined by:

$$\mathbb{D} = \mathbb{S}\mathbb{I}, \quad (2.72)$$

with  $\mathbb{I}$  being a column vector containing successively all the incident amplitudes  $\tilde{I}_{0,n}$  for  $n \in U_0$  and all the incident amplitudes  $\tilde{I}_{1,n}$  for  $n \in U_1$ ,  $\mathbb{D}$  being a column vector containing successively all the diffracted amplitudes  $\tilde{D}_{0,n}$ , and all the incident amplitudes  $\tilde{D}_{1,n}$  for  $n \in U_1$ . Thus, the order of column matrices  $\mathbb{I}$  and  $\mathbb{D}$  is the sum  $|U_0| + |U_1|$  of the cardinals of  $U_0$  and  $U_1$ . Using these notations, equation (2.71) can be expressed in the very simple form:

$$\langle \mathbb{D} | \mathbb{D}' \rangle = \langle \mathbb{I} | \mathbb{I}' \rangle, \quad (2.73)$$

the scalar product of two column matrices of order  $N$  being defined by:

$$\langle P | Q \rangle = \sum_{j=1}^N P_j \overline{Q_j}. \quad (2.74)$$

Using equation (2.72) to eliminate  $\mathbb{D}$  in equation (2.77) yields:

$$\langle \mathbb{S}\mathbb{I} | \mathbb{S}\mathbb{I}' \rangle = \langle (\mathbb{S}^* \mathbb{S}) \mathbb{I} | \mathbb{I}' \rangle = \langle \mathbb{I} | \mathbb{I}' \rangle, \quad (2.75)$$

with  $\mathbb{S}^*$  being the adjoint matrix of  $\mathbb{S}$ . Since equation (2.75) must be satisfied for any value of  $\mathbb{I}$  and  $\mathbb{I}'$ , we deduce that:

$$\boxed{\mathbb{S}^* \mathbb{S} = \mathbb{1}}, \quad (2.76)$$

with  $\mathbb{1}$  being the identity matrix. Equation (2.76) shows that  $\mathbb{S}$  is unitary.

### 2.5.3 Energy balance

The energy balance relation is obtain by taking  $u = v$  in equation (2.77), which gives:

$$\langle \mathbb{D} | \mathbb{D} \rangle = \langle \mathbb{I} | \mathbb{I} \rangle, \quad (2.77)$$

or equivalently:

$$\|\mathbb{D}\| = \|\mathbb{I}\|. \quad (2.78)$$

Let us show why this equation is known as energy balance relation. To this end, it suffices to use the Poynting theorem and to calculate the flux of the Poynting vector  $\vec{E} \times \vec{H}$  through the rectangle  $\Gamma_1 \Gamma_2 \Gamma_4 \Gamma_3$  of figure 2.2. Since the grating material is lossless, the flux of the Poynting vector through this rectangle (with now the normal oriented toward the exterior, in contrast with figure 2.2) must be null. The contributions of the vertical sides  $\Gamma_1 \Gamma_3$  and  $\Gamma_2 \Gamma_4$  cancel each other, thanks to the periodicity of the Poynting vector ( $\vec{H}$  has a coefficient of pseudo-periodicity which is the opposite to that of  $\vec{E}$ ). At the top of the rectangle, the calculation of the flux of the Poynting vector can be achieved by using the Rayleigh expansion given by

equations (2.64). Taking into account that  $\int_{x=0}^d \exp in \frac{2\pi}{d} x = \delta_n$ , elementary calculations show that the contributions to this flux of the different plane waves are decoupled and are proportional to  $-\gamma_{0,n}|I_{0,n}|^2$  and  $+\gamma_{0,n}|D_{0,n}|^2$ . At the bottom of the rectangle, we use the Rayleigh expansion given by equations (2.69). The contributions of the plane waves are decoupled as well and are proportional to  $-\frac{\tau_0}{\tau_1}\gamma_{1,n}|I_{1,n}|^2$  and  $+\frac{\tau_0}{\tau_1}\gamma_{1,n}|D_{1,n}|^2$ , with the same coefficient of proportionality as the contributions on the top of the rectangle. Therefore, the energy balance can be written:

$$\begin{aligned} \sum_{n \in U_0} \gamma_{0,n}|D_{0,n}|^2 + \sum_{n \in U_1} \frac{\tau_0}{\tau_1} \gamma_{1,n}|D_{1,n}|^2 = \\ = \sum_{n \in U_0} \gamma_{0,n}|I_{0,n}|^2 + \sum_{n \in U_1} \frac{\tau_0}{\tau_1} \gamma_{1,n}|I_{1,n}|^2. \end{aligned} \quad (2.79)$$

The first and second terms in the left-hand member of equation (2.79) represent the energy diffracted upwards and downwards respectively and the corresponding terms in the right-hand member are the incident energy propagating downwards and upwards respectively.

Coming back to the physical problem where the incident wave is unique and has a unit amplitude (see equation (2.26)), equation (2.79) becomes:

$$\sum_{n \in U_0} \gamma_{0,n}|D_{0,n}|^2 + \sum_{n \in U_1} \frac{\tau_0}{\tau_1} \gamma_{1,n}|D_{1,n}|^2 = \gamma_{0,0}, \quad (2.80)$$

the right-hand member representing the incident energy. In that case, the efficiency  $\rho_{i,n}$ ,  $i \in (0, 1)$  is defined as the ratio of the energy diffracted in a given order over the incident energy. Using equation (2.79) yields:

$$\rho_{i,n} = \begin{cases} \gamma_{0,n}|D_{0,n}|^2 & \text{if } i = 0, \\ \frac{\tau_0}{\tau_1} \gamma_{1,n}|D_{1,n}|^2 & \text{if } i = 1, \end{cases} \quad (2.81)$$

and the energy balance can be written:

$$\sum_{n \in U_0} \rho_{0,n} + \sum_{n \in U_1} \rho_{1,n} = 1. \quad (2.82)$$

**The sum of efficiencies is equal to unity.** When the grating is perfectly conducting, it is easy to show that the energy balance still holds, provided that the sum  $n \in U_1$  is cancelled in equations (2.79), (2.80) and (2.82). When the grating material is lossy, the sum  $n \in U_1$  must be cancelled as well and one can show that equation (2.82) becomes:

$$\sum_{n \in U_0} \rho_{0,n} < 1. \quad (2.83)$$

The sum of reflected efficiencies is smaller than one, a rather intuitive result if we bear in mind that a part of the incident energy is dissipated in the grating material.

#### 2.5.4 Reciprocity

In order to demonstrate the well known reciprocity relation, we consider a function  $u$ , sum of the solution of the normalized grating problem (see equations (2.28), (2.29), (2.30) and (2.31))

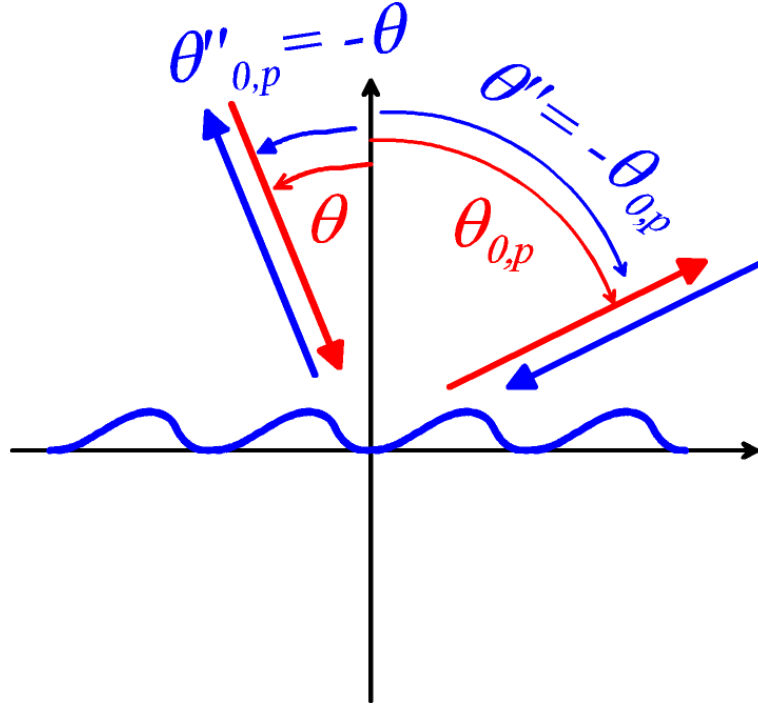


Figure 2.3: The reciprocity theorem: The efficiency in the  $p^{\text{th}}$  order is the same in the two cases symbolized by red and blue arrows.

and of the corresponding incident field (in other words,  $u$  is the total field). In order to define  $v$ , we consider the  $p^{\text{th}}$  order of diffraction ( $p \in U_0$ ) in  $\mathcal{R}_0$ , with diffraction angle  $\theta_{0,p}$ .

Then, we consider a second problem, but with angle of incidence  $\theta'' = -\theta_{0,p}$ , as shown<sup>3</sup> in figure 2.3. The incident wave in this second case has a direction of propagation which is just the opposite of that of the  $p^{\text{th}}$  diffracted order in the first case and straightforward calculations show that **the corresponding  $p^{\text{th}}$  order in  $\mathcal{R}_0$  has a direction of propagation which is the opposite of that of the incident wave in the first case**, which entails  $\theta''_{0,p} = -\theta$ . This geometrical property is known in optics as the reversion theorem. The constants of propagation of the  $p^{\text{th}}$  diffracted order in this second case are given by  $\alpha''_p = -\alpha_0$  and  $\gamma''_{0,p} = \gamma_{0,0}$  and more generally, the constants of propagation of an arbitrary  $n^{\text{th}}$  diffracted order in this second case are given by  $\alpha''_n = -\alpha_{p-n}$  and  $\gamma''_{0,n} = \gamma_{0,p-n}$ . Thus  $v''$  can be written:

$$v''(x, z) = \exp(-i\alpha_p x - i\gamma_{0,p} z) + \sum_{n=-\infty}^{+\infty} D''_{0,n} \exp(-i\alpha_{p-n} x + i\gamma_{0,p-n} z). \quad (2.84)$$

Functions  $u$  and  $v''$  do not satisfy the conditions of the equation of compatibility (equation (2.71)) since they have not the same pseudo-periodicity. It is not so for  $u$  and the function  $v = \overline{v''}$  which is given by:

$$v(x, z) = \exp(i\alpha_p x + i\gamma_{0,p} z) + \sum_{n=-\infty}^{+\infty} \overline{D''_{0,n}} \exp(i\alpha_{p-n} x - i\overline{\gamma_{0,p-n}} z). \quad (2.85)$$

<sup>3</sup>It must be remembered that the conventions for the measurements of the angles of incidence and diffraction in  $\mathcal{R}_0$  are opposite

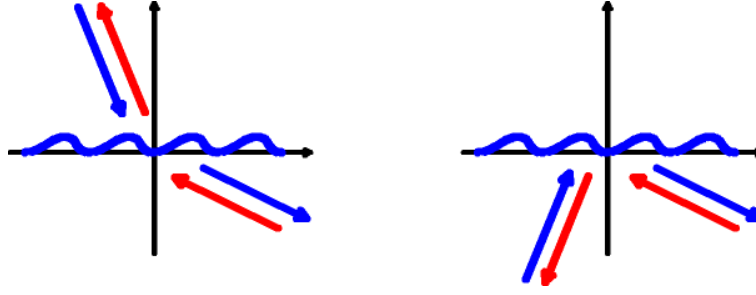


Figure 2.4: Other reciprocity relations: The efficiency is the same in the two cases symbolized by red and blue arrows.

Identifying the incident and diffracted waves in equation (2.85) yields:

$$I'_{0,n} = \overline{D''_{0,p-n}}, \quad (2.86a)$$

$$D'_{0,n} = \delta_{n-p}, \quad (2.86b)$$

and from equation (2.71), it turns out that:

$$\boxed{\gamma''_{0,p} D''_{0,p} = \gamma_{0,p} D_{0,p}} \quad (2.87)$$

**This is the reciprocity theorem: the products of the amplitudes of the plane waves represented in figure 2.3 by their propagation constants along the  $z$  axis is invariant.** In order to state the reciprocity theorem in a form which is most widespread, we take the modulus square of both members of equation (2.87):

$$\gamma''_{0,p}{}^2 |D''_{0,p}|^2 = \gamma_{0,p}{}^2 |D_{0,p}|^2. \quad (2.88)$$

Writing equation (2.88) in the form:

$$\frac{\gamma''_{0,p}}{\gamma_{0,p}} |D''_{0,p}|^2 = \frac{\gamma_{0,p}}{\gamma''_{0,p}} |D_{0,p}|^2, \quad (2.89)$$

and bearing in mind that  $\gamma_{0,p} = \gamma''_{0,0}$  and  $\gamma''_{0,p} = \gamma_{0,0}$ , and using the definition of the efficiencies given in equation (2.81), equation (2.89) yields:

$$\boxed{\rho''_{0,p} = \rho_{0,p}} \quad (2.90)$$

### The efficiency is invariant.

Figure 2.4 illustrates two other cases where the reciprocity theorem applies. These properties can be demonstrated by following the same lines as in the first part of this section. It is important to notice that the reciprocity theorem illustrated in figure 2.3 holds for lossy materials [9]. More surprisingly, the theorem can be generalized to evanescent waves [10].

#### 2.5.5 Uniqueness of the solution of the grating problem

If two different solutions of the normalized grating problem exist, their difference  $w(x, z)$  does not include any incident wave. We will show that such a field vanishes. We assume here that the

grating material is lossless. First, using the compatibility equation (2.71) with  $u = v = w$ , it emerges that:

$$\frac{1}{\tau_0} \sum_{n \in U_0} \gamma_{0,n} |D_{0,n}|^2 + \frac{1}{\tau_1} \sum_{n \in U_1} \gamma_{1,n} |D_{1,n}|^2 = 0. \quad (2.91)$$

Since  $\tau_0$ ,  $\tau_1$ ,  $\gamma_{0,n}$  and  $\gamma_{1,n}$  are positive, equation (2.91) implies that  $D_{0,n} = D_{1,n} = 0$ . This is an important result since it means that if  $w$  exists, it has no effect on the far field: the solution in the far field is unique. However, it could exist a function  $w$  localized at the vicinity of the grating profile and tending to zero exponentially at infinity. The interested reader can find a complete and not straightforward demonstration of the uniqueness in [1], at least for the TE case.

### 2.5.6 Analytic properties of crossed gratings

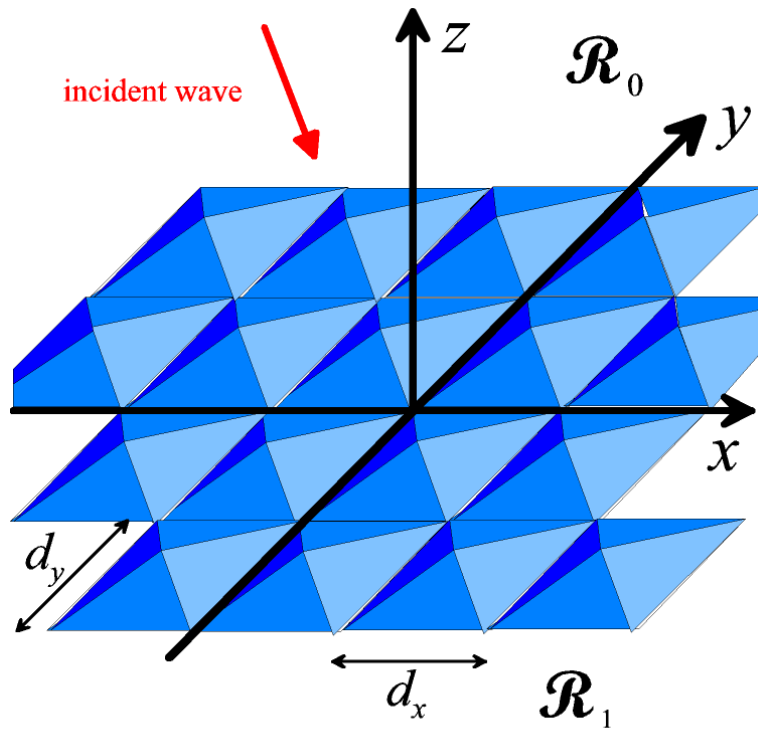


Figure 2.5: A crossed grating with periods  $d_x$  and  $d_z$  on the  $x$  and  $z$  axes.

Now, we consider the diffraction problem schematized in figure 2.5. An incident wave of wavevector  $\vec{k}_0$  is incident on a doubly-periodic structure separating air (region  $\mathcal{R}_0$ ) from a grating material (region  $\mathcal{R}_1$ ). We use all the notations defined in the preceding sections to characterize the materials. The incident field is schematized in figure 2.6. The direction of incidence is specified by the polar angles  $\Phi$  and  $\Psi$  (see figure 2.6). In order to define the polarization of the incident field, we construct the circle  $MNM'N'$  in the plane perpendicular to  $\vec{k}_0$ , with the continuation of  $NN'$  intersecting the  $z$  axis and  $MM'$  being perpendicular to  $NN'$ . The polarization angle  $\delta$  is the angle between  $M'M$  and the direction of the incident electric field  $\vec{P}$ . With these notations, the incident electric field is given by:

$$\vec{E}^i = \vec{P} \exp(i\alpha x + i\beta y - i\gamma z), \quad (2.92)$$



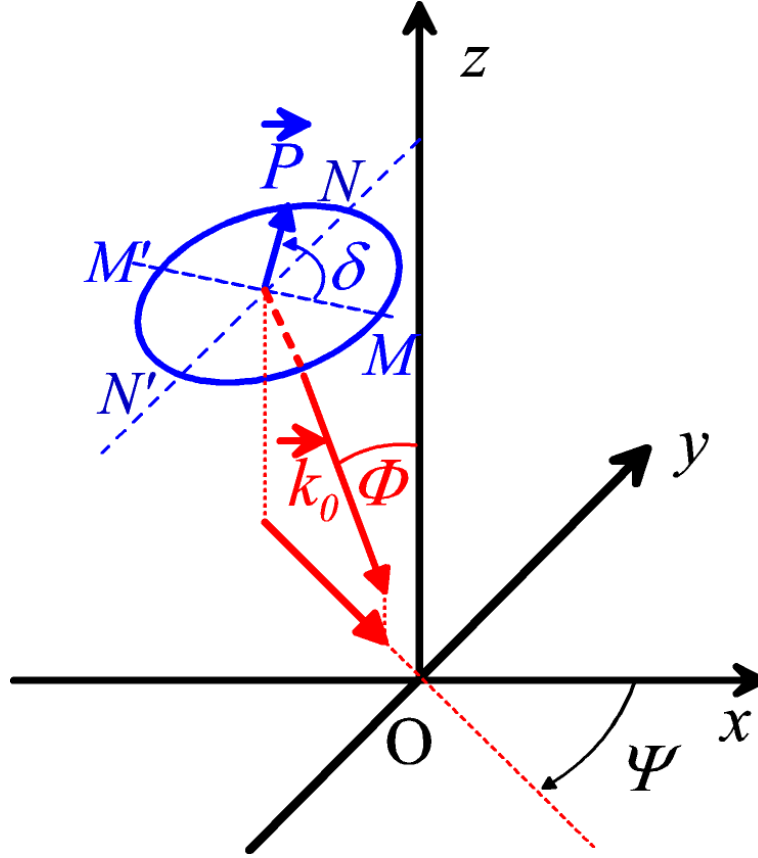


Figure 2.6: Notations for the incident field.

with  $\alpha = k_0 \sin \Phi \cos \Psi$ ,  $\beta = k_0 \sin \Phi \sin \Psi$  and  $\gamma = k_0 \cos \Phi$ . The projection of  $\vec{P}$  on  $M'M$  is called transverse component of  $\vec{P}$  and denoted by  $P^t$ . Its projection on  $N'N$  is called longitudinal (in plane) component and denoted  $P^l$ , in such a way that  $\vec{P} = P^t \frac{\overrightarrow{MM'}}{MM'} + P^l \frac{\overrightarrow{NN'}}{NN'}$ .

As in the case of classical gratings, it is possible to show that above the top of the grating ( $z > z_M$ ), the field can be expanded in the form of a sum of plane waves:

$$\vec{E}(x, z) = \begin{cases} \sum_{n=-\infty}^{+\infty} \sum_{m=-\infty}^{+\infty} (\overrightarrow{I_{0,n,m}} \exp(i\alpha_n x + i\beta_m y - i\gamma_{0,n,m} z) + \\ \quad + \overrightarrow{D_{0,n,m}} \exp(i\alpha_n x + i\beta_m y + i\gamma_{0,n,m} z)), & \text{if } z > z_M, \\ \sum_{n=-\infty}^{+\infty} \sum_{m=-\infty}^{+\infty} (\overrightarrow{D_{1,n,m}} \exp(i\alpha_n x + i\beta_m y - i\gamma_{1,n,m} z) + \\ \quad + \overrightarrow{I_{1,n,m}} \exp(i\alpha_n x + i\beta_m y + i\gamma_{1,n,m} z)) & \text{if } z < 0. \end{cases} \quad (2.93)$$

The wavevectors of all these plane waves must be orthogonal to their vector amplitudes. As for the incident wave, we can define the transverse and longitudinal components of the vector amplitudes of the plane waves, the transverse component (for example  $\overrightarrow{D'_{0,n,m}}$ ) being orthogonal to the  $z$  axis in the plane perpendicular to the wavevector  $(\alpha_n, \beta_m, \gamma_{0,n,m})$  and the longitudinal (for example  $\overrightarrow{D^l_{0,n,m}}$ ) its component in the orthogonal direction of the same plane.

Using the Poynting theorem, it can be shown, as in section 2.5.3, that the efficiencies in the  $z$ -propagating orders are given by:

$$\rho_{i,n,m} = \begin{cases} \frac{\gamma_{0,n,m}}{\gamma_{0,0}} |\overrightarrow{D}_{0,n,m}|^2 & \text{if } i = 0, \\ \frac{\gamma_{1,n,m}}{\gamma_{0,0}} \left( \frac{1}{v^2} |D^l_{1,n,m}|^2 + |D^t_{1,n,m}|^2 \right) & \text{if } i = 1. \end{cases} \quad (2.94)$$

Of course, the line associated to  $i = 1$  in equation (2.94) must be cancelled if the grating material is lossy.

We define, as for classical gratings, the sets  $U_0$  and  $U_1$  of  $z$ -propagating orders in  $\mathcal{R}_0$  and  $\mathcal{R}_1$  respectively and, when the grating material is lossless, the energy balance can be written:

$$\boxed{\sum_{(n,m) \in U_0} \rho_{0,n,m} + \sum_{(n,m) \in U_1} \rho_{1,n,m} = 1.} \quad (2.95)$$

We will not demonstrate the reciprocity theorem, the interested reader can find the proof in [1]. This theorem, in the case of an order  $(p, q)$  propagating in  $\mathcal{R}_0$  can be expressed in the following form:

$$\boxed{\gamma \vec{P} \cdot \vec{D}'_{0,p,q} = \gamma' \vec{P}' \cdot \vec{D}_{0,p,q}.} \quad (2.96)$$

In the first case, the incident electric field with vector amplitude  $\vec{P}$  and propagation constant along the  $z$  axis  $-\gamma$  generates in  $\mathcal{R}_0$  in the  $(p, q)$  order, with  $(p, q) \in U_0$ , a plane wave of vector amplitude  $\vec{D}_{0,p,q}$  and propagation constant along the  $z$  axis  $\gamma_{0,p,q}$ . In the second case, we consider an incident wave which propagates in the direction which is just the opposite to that of the  $(p, q)$  order in the first case. Thus its constant of propagation along the  $z$  axis is  $-\gamma' = -\gamma_{0,p,q}$ . The vector amplitude of this incident wave is equal to  $\vec{P}'$ . It can be shown that in this second case, the  $(p, q)$  order takes the direction which is the opposite of that of the incident wave in the first case and its vector amplitude is equal to  $\vec{D}'_{0,p,q}$ . **Thus, equation (2.96) can be expressed in the following form: the scalar product of the vector amplitudes of the incident and diffracted waves propagating in the opposite directions, multiplied by the propagation constant of the incident wave along the  $z$  axis, is constant.** It can be shown that this relation entails the **reciprocity in natural light for the efficiencies**:

$$\boxed{\langle \rho_{0,p,q} \rangle = \langle \rho'_{0,p,q} \rangle,} \quad (2.97)$$

with  $\langle \rho_{0,p,q} \rangle$  being the average between the efficiencies in both cases of polarization ( $\delta = 0$  and  $\delta = \frac{\pi}{2}$ ).

## 2.6 Conclusion

We have established the mathematical bases of grating theories: the boundary-value problems. Most of the formalisms used for solving the grating problems numerically start from these boundary-value problems, for example the integral theory [1,2]. Other theories use some conditions of these problems but deal directly with Maxwell equations, for example the RCWA method [5].

Without any doubt, the boundary-value problems are necessary to demonstrate the analytic properties of gratings. Very often, these properties are ignored or neglected. However, properties like energy balance or reciprocity are needed for a full understanding of the puzzling properties of this crucial component of optics and nanophotonics. These analytic properties are also widely used to check new grating softwares. However, they are not more than casting out nines. They can show that a software fails if they are not satisfied on its numerical results. It must be emphasized that they can never prove its validity if they are satisfied.

Some important analytic properties of gratings have not been mentioned in this chapter. It is the case for example for the Marechal and Stroke theorem, the only grating property which allows one to know the field diffracted by a grating without any calculation. This theorem, which is restricted to perfectly conducting echelette gratings used for TM polarization in very special conditions will be given in the chapter devoted to the applications of grating properties.

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